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The prediction and verification of CO production rate based on extended mixture-fraction method

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Abstract

The paper uses both single-step and two-step reaction models to predict the yield of CO in a standard room with the half size of ISO9705 under different ventilation situations, and verify the validity of calculation results with the comparison against experimental data. The results show that the two-step combustion model can predict the yield of CO more precisely as long as under a proper grid and boundary setup. In practical researches of human evacuation and toxic gases, the method of FDS5 simulation can be used to predict gas yields which can do practical instructions.

Peer-review under responsibility of the organizing committee of ICPFFPE 2015

Keywords: *Extended mixture fraction model; CO yield; ventilation variation*.

Nomenclature

D	diffusion coefficient
D/Dt	substantial derivative
f_i	the normalized yield of species i
f	the sum of the normalized yield of carbon-containing products
k_i	the theoretical maximum yield of species i
m_i	the mass of species i (kg i)
$\dot{m}_i$	the mass flow of species i (kg i/s)
$\dot{m}_i'''$	the species i production rate (kg i/m^{3}s)
r	the stoichiometric ratio of fuel to air
R	universal gas constant
t	time(s)
T	temperature(K)
W_i	molecular weight of species i (kg i/kmol i)
X_H	hydrogen atom fraction

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Y_i	mass fraction of species i (kg i/kg)
Y_i^I	fuel inlet mass fraction of species i (kg i/kg)
Z_i	mixture fraction component
Greek symbols	
ϕ	equivalence ratio
ρ	density (kg/m^3)
v_i	stoichiometric coefficient of species i
v_{co}	fixed yield stoichiometric coefficient of CO
$v_{co}^{'}$	stoichiometric coefficient of CO

1. Introduction

Fire Dynamics Simulator (FDS) developed by the National Institute of Standards and Technology (NIST) is widely used in the area fire simulation, which, for large-size experiments, generally uses a mixture-fraction model to reduce the number of transport equations and to decrease the calculation work. Mixture-fraction is a function of time and space, expressed by the sign of Z(x, t).The single component has something to do with the mixture-fraction. FDS2 and FDS4 consider that the gas component is determined by mixture-fraction, assuming that the mixed fuel and oxygen can react on the flame front instantly. However, the single mixture-fraction model is lack of some extra scalar parameters, which means that the CO production situation under incomplete combustion can't be completely simulated.

For ventilation control combustions, even as the fuel and the oxygen have mixed, there is still probability of non-reaction.

FDS5 takes a restraining single-step reaction model into consideration. It divided the mixture fraction, Z, into two parts: the burned fuel, Z1, and the unburned fuel, Z2. By assuming the production rates of CO and soot are both constant, this method is used to explain the fuel and the oxygen that do not react. There are two reaction processes: the first process is a empty reaction where the fuel and the oxygen mix without combustion reaction, while the second one is complete reaction where the fuel and the oxygen react, yielding products. During the solving process, the transport equations about Z1 and Z2 need to be solved. On the flame front, Z1 is the mass flow rate of fuel and Z2 is 0. The mass fraction of products is linear combination of Z1 and Z2.The local heat release rate is determined by the rate of fuel transforming into products directly.

Although the one-step model which considers the combustion restrain has been advanced, it is still not precise to forecast the production rate of CO when under the ventilation control situation. Based on the advantage of reducing calculation time of mixture fraction combustion model, the extended mixture fraction is used in the paper to explain the uncomplete combustion phenomenon to overcome its limitation.

FDS5 adds two-steps reaction model to predict the fire when ventilation is limited [1].

The first step: Fuel+O2→CO + other products

The second step: CO+1/2O2→CO2

So the specific reaction is as following:

$$\begin{aligned} &CxHyOzNaMb + v_{O_2} O_2 \rightarrow v_{H_2O} H_2O + (v'_{CO} + v_{CO})CO + v_s soot + v_{N2} N_2 + v_M M \\ &v'_{CO}(CO + 1/2O_2) \rightarrow v'_{CO}\, CO_2 \end{aligned} \tag{1}$$

The FDS5 has single-step reaction and two-step reaction models. The single-step reaction determines the yields of CO and soot directly. While in the two-step reaction models, the first step is a rapid reaction process. If the fuel and the oxygen and the CO are in a grid admitted to combust at the same time, the second step will proceed following the first step closely, and if there is sufficient amount of oxygen presented, and the heat release rate does not reach the upper limit, the CO will convert into CO2 immediately. Away from the flame, a finite-rate reaction computation is performed to convert CO to CO2.

The equation is as following [2]:

$$k(T) = 2.53*10^{12} e^{-199.547/RT} \tag{2}$$

To describe the composition of the gas species, the mixture fraction, Z, is decomposed into 3 components which are the unburned fuel, the CO yielded in the first step and the CO_2 converted in the second step [3].

$$Z_1 = \frac{Y_F}{Y_F^I} \tag{3}$$

$$Z_2 = \frac{W_F}{[x-(1-X_H)v_s]W_{CO}} * \frac{Y_{CO}}{Y_F^I} \tag{4}$$

$$Z3 = \frac{W_F}{[x-(1-X_H)v_s]W_{CO_2}} * \frac{Y_{CO_2}}{Y_F^I} \tag{5}$$

It is indicated that Z=Z1+Z2+Z3. The following transport equations were derived for these three mixture fraction variables:

$$\frac{DZ1}{Dt} = \nabla \cdot D\rho\nabla Z1 + \dot{m}'''_{F,1} \tag{6}$$

$$\frac{DZ2}{Dt} = \nabla \cdot D\rho\nabla Z2 - \dot{m}'''_{F.1} + \frac{W_F}{v_{CO}W_{CO}}\dot{m}'''_{CO,2} \tag{7}$$

$$\frac{DZ3}{Dt} = \nabla \cdot D\rho\nabla Z3 - \frac{W_F}{v_{CO}W_{CO}}\dot{m}'''_{CO,2} \tag{8}$$

J.E. Floyd compared experimental results and FDS simulation results under different ventilation situations, and verified that on the concentrations of CO and CO2, and the temperature, the two-step reaction model is accurate. The paper predicts and verifies the yield of CO under various ventilation situations by using single-step and two-step reaction models respectively.

2. Experiment

The test is carried out in a standard room of the half size of ISO9705, and the test compartment is as shown in Fig. 1. The room size is 1.22m wide, 1.78m long, and 1.17m high, inside which there is a 25.4mm thick ceramic plate. To achieve different ventilation conditions, the room opening is set with different width, and this article selects the width of 0.076m. The different ventilation situations can be reached through the room opening with different width. The paper choses a 0.076m width to test. In order to form the smoke layer, the upper part of the door opening is designed with an arch soffit of 0.4m high. The fuel is gaseous propane. The burner is of a 0.305m diameter and a 0.102m height. The fire power used to simulate is 91Kw, 204Kw, 264Kw and 379Kw respectively. The size of simulation area is 2.5m*1.5m*1.5m. The size of grids is 0.02m*0.02m*0.02m and the number of which is 360000. The simulation time is set as 300s.

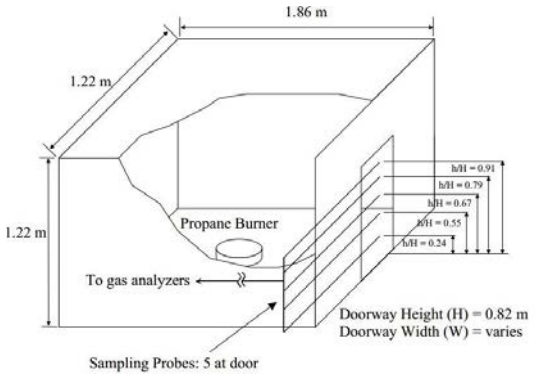

Fig. 1. Schematic of test device in 1/2 ISO9705

3. Results and Discussion

For the fires in the compartment, the yields of CO in a single-step reaction can be predicted through Gottok's empirical equations [4]:

$$Y_{CO} = (0.22/180)\tan^{-1}(10(\phi - 1.25)) + 0.11 \tag{9}$$

$$\phi = \frac{\dot{m}_f / \dot{m}_a}{r} \tag{10}$$

Where Φ is the equivalence ratio, $\dot{m}_f$ and $\dot{m}_a$ are the fuel mass flow rate and the air flow rate into room respectively. r is the stoichiometric ratio of fuel to air.

The normalized yield, f_i , is calculated by dividing the species yield by the maximum theoretical yield[2]:

$$Y_i = \frac{m_i}{m_f} \tag{11}$$

$$f_i = \frac{Y_i}{k_i} \tag{12}$$

$$f = f_{co} + f_{co_2} + f_{soot} = 1 \tag{13}$$

Where m_f , the mass flow difference between the evaporated fuel and the non-reaction fuel flowing out the room, is the mass of reaction fuel, and m_i is the mass flow of species i . k_i and f_i denotes the theoretical maximum yield and the normalized yield of species i respectively, and f is the sum of the normalized yield of carbon-containing products. The conservation of carbon requires that f is equal to unity. For propane, $k_{co} = 1.91$.

The single-step reaction of 91Kw is taken as an example to find a solution of yield of CO, and the unburned gas and the gross evaporated gas are as shown in Fig. 2. The actual fuel in reaction is the difference of the both fuels above. And the combustion flow of the actual fuel in stable phase is 0.00192Kg/s.

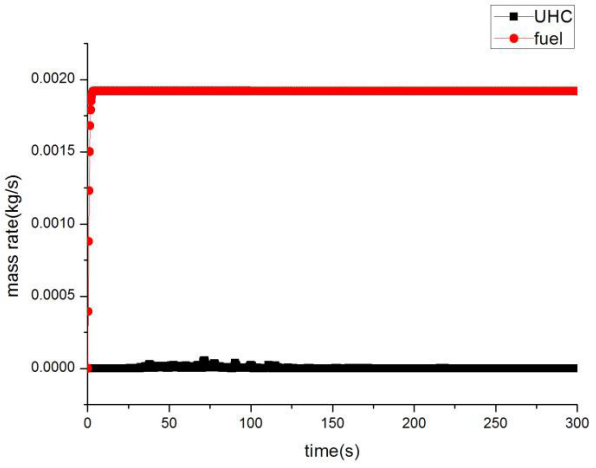

Fig. 2. Mass flow of the unburned gas and the gross evaporated gas

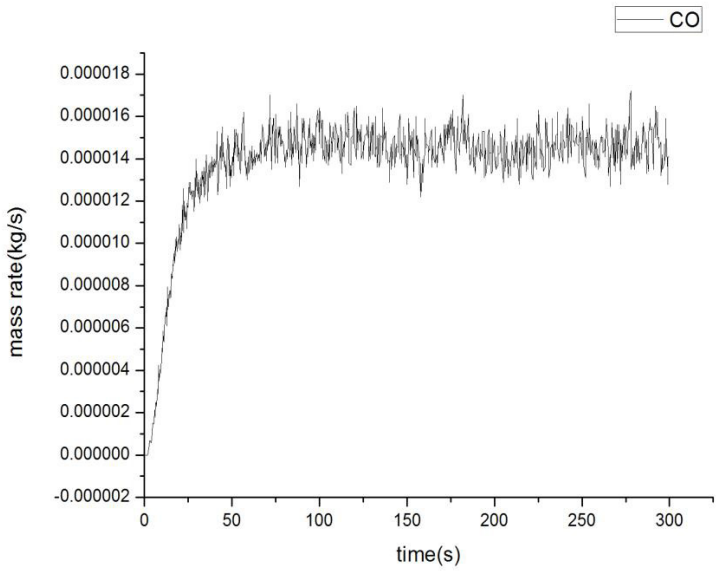

Fig. 3. Mass flow of CO under the fire power of 91Kw

The yield of CO is 1.4571e-5Kg/s, as shown in the Fig. 3. So the mass fraction and the normalized yield of CO are as followings:

$$Y_{CO} = \frac{1.4571\text{e-}5}{0.00192} = 0.007 \tag{14}$$

$$f_{CO} = \frac{Y_{CO}}{k_{CO}} = \frac{0.007}{1.92} = 0.00364 \tag{15}$$

For other test conditions, the same calculation method is used, and then both the single-step and two-step predictions of the mass fraction of CO under various fire powers of 91Kw, 204Kw, 264Kw and 379Kw are compared against measured data from the tests, which is as shown in the Table 1 and the Fig. 4. A period of 60s is taken as the stable phase to get the average value, consistent with the method in tests. The measured deviation of the yield of CO is 51.8%.

Table 1. Mass fractions of CO with both single-step and two-step reaction under various fire powers

The fire power(Kw)	Single-step reaction Y_{co}	Two-step reaction Y_{co}	Test data Y_{co}
91	0.007	0.00476	0.00998±0.00517
204	0.0157	0.1688	0.13758±0.0713
264	0.0581	0.4135	0.37096±0.1926
379	0.2012	0.5853	0.50241±0.2602

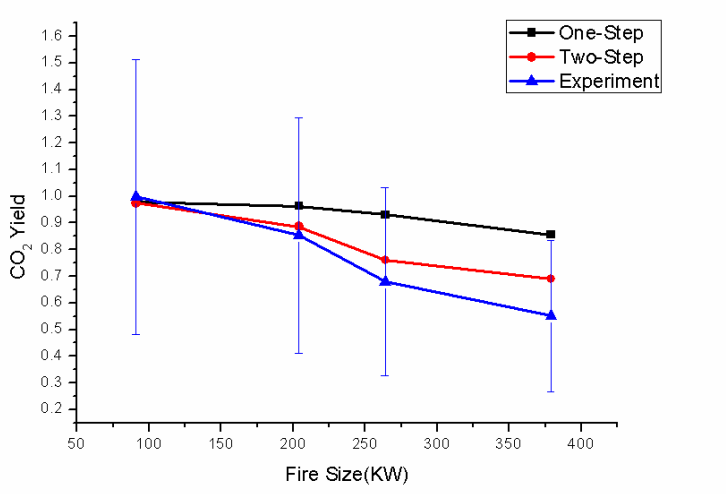

Fig. 4. Comparison of both single-step and two-step predictions against test measured data of the yield of CO

Fig.4.shows that with the consideration of tests' measured deviation, the two-step reaction model does a better prediction on the yield of CO. For single-step reaction model, the prediction is only roughly consistent with the test data under a good ventilation situation. With the increase of fire power, which means the reduction of oxygen, the yield of CO is lower than the real data. While for two-step reaction model, although the yield of CO is higher, it is closer to the test data. This is mainly due to that the simulation program does an integration to the CO of the whole outlet, while the test yield of CO depends on the solution of the gas flowing out above the neutral surface. In the tests, the concentration of lower smoke layer is small, so the deviation is correspondingly small.

Although there are some shortages in the two-step reaction model, like the designation of burning areas and the easy empirical criterion based on oxygen concentration and flame temperature, and in addition, the first step reaction is still a infinitely fast process without the external control, while in some real cases, like in a low temperature and low-density oxygen surrounding, the production rate of CO is pretty slow, it is still more advanced on the yield prediction than the single-step model. Fig.5.shows that when the temperature gets to 800K, the prediction will higher because of the poor oxygen [4].

Above all, the two-step reaction prediction is acceptable under both good and bad ventilation situations when the proper grids and boundary condition are set.

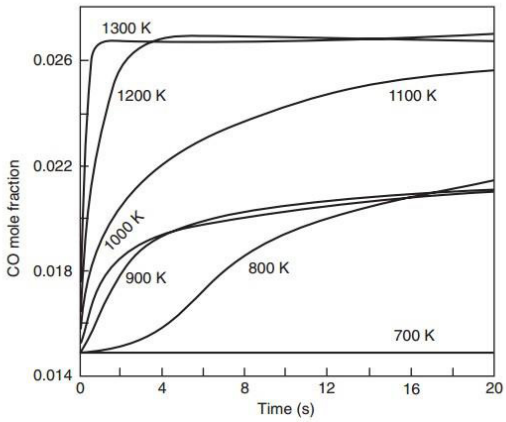

Fig. 5. The CO concentration versus time at adiabatic conditions. Initial concentrations from a methane hood fire at $\phi = 2.17$.

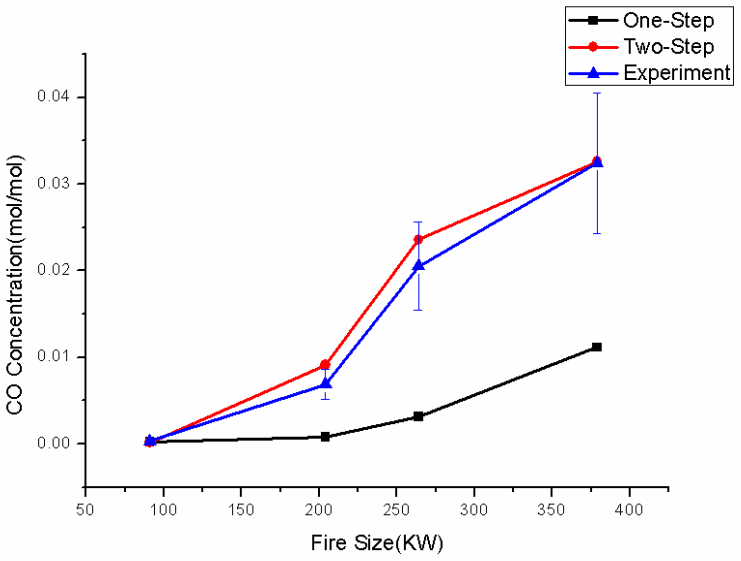

Fig. 6. Comparison of both single-step and two-step predictions against test measured data of the average mole concentration of CO

The slicing of the volume fraction of CO is set at the opening, the information of which is then transformed into text file through fds2ascii.exe. By analysing the slicing information, the average mole concentration of CO above neutral surface is solved and compared against the test data, as shown in the Table 2 and Fig.6.

Table 2. Mass fractions of CO with both single-step and two-step reaction under various fire powers

The fire power(Kw)	Single-step reaction VF_{co}	Two-step reaction VF_{co}	Test data VF_{co}
91	0.00022	0.000137	0.000338±0.0000845
204	0.0008	0.0091	0.0068846±0.00172
264	0.003145	0.0236	0.020547±0.0051
379	0.01115	0.0326	0.032443±0.00811

Fig.6.shows that with the consideration of measured deviation, the two-step reaction model does a better prediction on average mole concentration under both good-bad ventilation situations, while as the increase of fire power, the single-step reaction prediction is lower.

4. Conclusion

The paper simulates the fire in a proportionally reduced compartment under different ventilation situations by using the two-step combustion model and the one-step model respectively, showing that in the fuel control phase, the two models can either do valid predictions, while, when in the ventilation control phase, although the yield of CO is higher, the two-step combustion model does a closer prediction of the production and consumption of CO by decomposing the mixture fraction into non-reaction fuel, incomplete reaction yield of CO in the first step reaction and complete converted yield of CO_2 in the second step reaction. For single-step reaction model, the prediction is only roughly consistent with the test data under a good ventilation situation. With the increase of fire power, which means the reduction of oxygen, the yield of CO is lower than the real data.

Under the setup of proper grids and boundary conditions, the deviation between predictions and test data is in a reasonable range.

Acknowledgements

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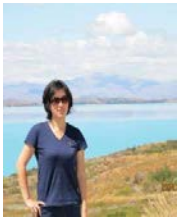
Appendix A. About the Authors

Ruxue Kang, who born in Xian Yang, Shann Xi province in 24, 11, 1992, is a master candidate of State Key Laboratory of Fire Science (SKLFS) of USTC, Hefei, China. She received a bachelor of safety engineering degree from Xi'an University of Architecture and Technology, China, in 2010. Now she is focusing her research on fire extinguishment. 26mm in width and 32mm in height.



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